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14. ABSTRACT Competition between unimolecular decomposition of highly energetic azabenzene molecules and relaxation via collisions with bath molecules is investigated to provide insight to the dynamics of prototypical explosive materials. High energy azabenzene molecules (4-5 eV) are prepared with pulsed tunable UV excitation and the resulting energy loss processes are monitored using high resolution transient infrared absorption spectroscopy. Nascent energy gain measurements in bath molecules such as CO ₂ and H ₂ O provide information about the energy transfer partitioning, cross sections and distribution functions. Computer simulations using classical trajectory calculations help identify the molecular features that lead to efficient (or inefficient) energy loss pathways.					
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Objective

The objective of Mullin's research is to investigate collisional energy flow and chemical reactivity of highly excited nitrogen-containing molecules that serve as prototypes for secondary explosives in energetic environments. Experimental techniques are developed to identify the predominant energy loss pathways, quantify the nature and efficiencies for such pathways, explore the energy dependent energy loss processes and develop an understanding at the molecular and intermolecular level for the observed energy dissipation processes.

Approach

Highly vibrationally excited azabenzenes are prepared in low-density gas-phase environments using tunable pulsed UV laser excitation, followed by rapid radiationless decay to the ground electronic state. The excited azabenzenes are prepared with well-defined initial vibrational energy between 31,000 to 41,000 cm^{-1} . Energy loss caused by collisions of the hot azabenzenes with surrounding cool molecules is investigated by probing the energy gain into individual quantum states of the bath using high-resolution transient IR laser absorption. Absorption measurements for IR wavelengths greater than 3.3 microns are made using a cw liquid-nitrogen cooled diode laser and for shorter IR wavelengths, a scanning single-mode F-center laser is used. Nascent rotational populations are measured using transient IR absorption. Measurements of Doppler-broadened transient absorption lineshapes provide information about the nascent distributions of recoil velocities of the bath molecules. These data provide insight into the dynamics of energy loss pathways and absolute rate measurements yield information on state-resolved quenching efficiencies. Competition with unimolecular decomposition is investigated through IR probing of reaction products.

Progress

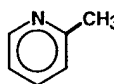
A. **Summary of completed work.** The research activities in Mullin's group have focussed on the collisional behavior of highly excited azabenzene molecules, which are shown below. These



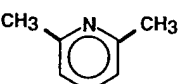
Pyrazine



Pyridine



2-Picoline



2,6-Lutidine

nitrogen containing molecules are prototypes for secondary explosives. They are particularly interesting in exploring the behavior of these molecules when they contain large amounts of internal energy. Their approach to these studies is

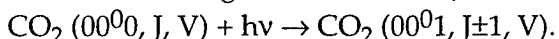
to investigate the energy flow from the hot molecules by monitoring the *energy gain* in the surrounding bath molecules, rather than focusing on the hot donors themselves. They use nanosecond UV excitation to prepare highly excited molecules having well-defined energies between 30000 and 42000 cm^{-1} , and they use high-resolution transient IR absorption to monitor population changes in individual quantum states of bath molecules. The Mullin lab monitors population changes in the bath states at short times relative to bulk collisions to get information about the scattered bath molecules immediately after a collision. This combination provides them the unique ability to identify the salient energy flow pathways and to measure the effect of internal energy on the vibrational, rotational and translational energies of the bath molecules after collisions with high-energy nitrogen-containing donor molecules. Through these studies, Mullin and her group have addressed three important facets of the collisional deactivation dynamics. In particular, they have studied how the relaxation dynamics are influenced by 1) the complexity of the donor molecule, 2) the energy content of the donor molecule, and 3) the structure of the acceptor species. In addition, they have begun a joint theoretical effort with Prof. David Coker using classical trajectory methods to model collisional energy loss dynamics in highly excited azabenzenes. Here their major findings in each of these areas are described.

The role of donor complexity in strong collisions: Bulk measurements of energy loss from excited donors, which have been performed in other groups over the past 15 years, show that the average energy loss from highly excited molecules increases as the complexity of the hot donor increases. However, little is known about the specific energy flow pathways that are responsible for these observations. In the Mullin labs, high-resolution transient IR absorption probing of the bath molecules is used to determine how energy flows from the hot donor into the vibrational, rotational and translational degrees of freedom of the acceptor molecule. They have used this approach to investigate the ways in which molecular complexity of the donor influences the energy loss dynamics for the highly excited donor molecules shown above. Their studies of donor complexity have focused on how "supercollisions" are influenced by the number of vibrational modes in the excited azabenzene donor molecule. "Supercollision" energy transfer refers to impulsive collisions that exchange large amounts of energy, which they take here to be greater than ~ 10 kT. This type of energy transfer corresponds to the high energy tail of the energy transfer distribution function, $P(E,E')$. Such phenomena have been observed for collisions of highly excited pyrazine ($E=41000\text{ cm}^{-1}$) with CO_2 , in which as much as 9000 cm^{-1} are exchanged in a single collision. These encounters leave CO_2 with excessive rotational and translational energy, but are not accompanied by CO_2 vibrational excitation. Thus, observation of energy flow into CO_2 rotation and translation is a sensitive measure of the high energy tail of $P(E,E')$ for different donor molecules.

In a typical experiment, highly excited donor molecules are generated by pulsed ($t \sim 7$ ns) UV absorption of $\lambda=266$ nm light from the quadrupled output of a Nd:YAG laser. Radiationless decay to the ground electronic state transforms the photon energy ($E=38000\text{ cm}^{-1}$) into vibrational energy with a lifetime that is much shorter than that for energy transfer under our experimental pressure of 20 mTorr. For this strong collision process, collisions with CO_2 molecules remove energy from the hot donors,



resulting in excited CO_2 , where (00^0_0) refers to the vibrationless ground state, J is rotational angular momentum quantum number, and V is the projection of the recoil velocity along the IR probe axis. The appearance of individual quantum states of the scattered CO_2 molecules is measured by transient IR absorption of a single-mode diode laser using the strongly-allowed ν_3 antisymmetric stretching transition at $4.3\text{ }\mu\text{m}$,



Probing individual transitions is possible due to the high spectral purity of the IR laser ($\Delta\nu \sim 0.0003\text{ cm}^{-1}$). Nascent velocity distributions of the scattered CO_2 molecules are determined by measuring the Doppler-broadened absorption lineshapes for different transitions. All population and lineshape measurements are made at short times ($1\text{ }\mu\text{s}$) following the UV pulse so that contributions from multiple collisions are minimized.

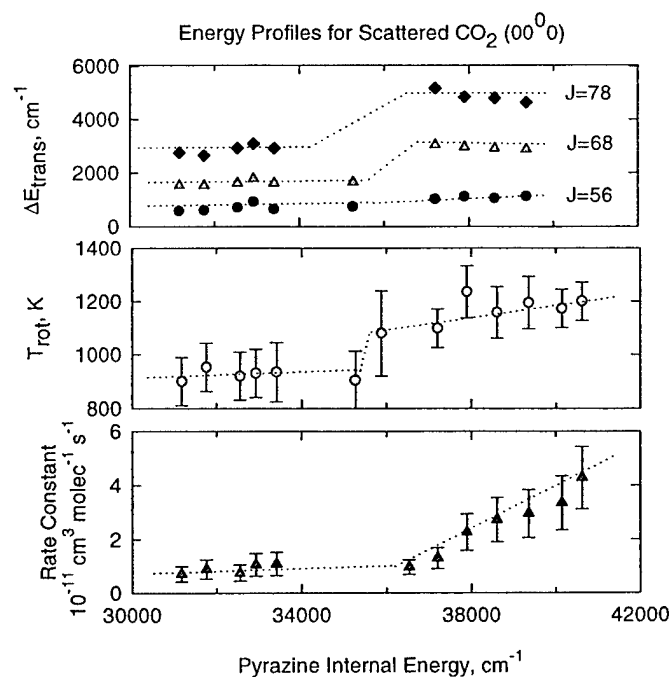
Mullin's group has measured the energy profiles for $\text{CO}_2(00^0_0)$ molecules that result from collisions with highly excited pyrazine, pyridine, 2-picoline and 2,6-lutidine at $E=38000\text{ cm}^{-1}$. Their data show that significant rotational and translational excitation of $\text{CO}_2(00^0_0)$ occurs for each of the excited donors. Most strikingly, pyrazine, with the smallest number of vibrational modes, is responsible for the largest CO_2 energy gains ($T_{\text{rot}}=1100\pm 150\text{ K}$ and $T_{\text{trans}}\sim 2000\text{--}4000\text{ K}$ for $J=56\text{--}84$) while the most complex of the donors, 2,6-lutidine, is responsible for the smallest CO_2 energy gains ($T_{\text{rot}}=530\pm 70\text{ K}$ and $T_{\text{trans}}\sim 1000\text{--}2000\text{ K}$ for $J=56\text{--}80$). Intermediate values of CO_2 energy gain are observed for pyridine and 2-picoline. These data are a clear indication that the impact felt by CO_2 is diminished when the donor's internal energy content is spread among

more internal degrees of freedom. This is consistent with our expectation that molecules with greater complexity are better able to store internal energy, since that energy will rapidly diffuse through the available phase space. In contrast, they find that the energy transfer rates for the strong collisions of 2,6-lutidine are eight times greater than for those of pyridine. These data provide a clear picture of how molecular complexity influences the strong collisions that deactivate hot azabenzene molecules. In these systems, the great majority of supercollisions occur via close-range impulsive interactions. This would suggest that high amplitude, high energy motions of the donor molecules are responsible for these supercollisions. These ideas provide a natural explanation for the results of their donor complexity experiments. Activated molecules with greater complexity undergo smaller amplitude and lower energy fluctuations because they are better able to spread the energy among the available modes. Thus, the more complex hot donors are able to impart less recoil to the acceptor. Interestingly, it appears that for the more complex molecules in this study, energy transfer is more likely to occur. Whether this arises from the influence of target size, increased floppiness due to methyl substitution or some other effect remains to be determined.

The role of donor energy content: Supercollision thresholds and resonant vibrational excitation: Bulk collision studies report that average energy loss per collision increases monotonically with the internal energy of the excited donor. In the Mullin lab, they have coupled high-resolution IR probing of energy gain in the bath with tunable UV excitation of complex donor molecules to provide the first direct measurements of the ways in which a polyatomic molecule's internal energy influences its collisional relaxation pathways. At energies approaching the dissociation threshold, the excited molecule is expected to experience large amplitude excursions from its equilibrium structure, which in turn may have significant impact on its energy transfer dynamics. Thus, by preparing donor molecules with a range of well-defined internal energies, detailed information about this interesting region of the potential energy surface can be obtained.

Mullin and her group have performed extensive energy-dependent studies on rotational and translational energy gain in the CO_2 (00^0_0) state resulting from collisions with excited pyrazine. In these experiments, pyrazine molecules, Pyr(E), are generated with internal energies of $E_{\text{vib}} = 30000\text{--}42000\text{ cm}^{-1}$ by pulsed UV excitation from either the tripled output of a Nd:YAG-pumped Ti:sapphire laser ($\lambda = 245\text{--}280\text{ nm}$) or the doubled output of a Nd:YAG-pumped dye laser ($\lambda = 285\text{--}330\text{ nm}$) and CO_2 energy gain

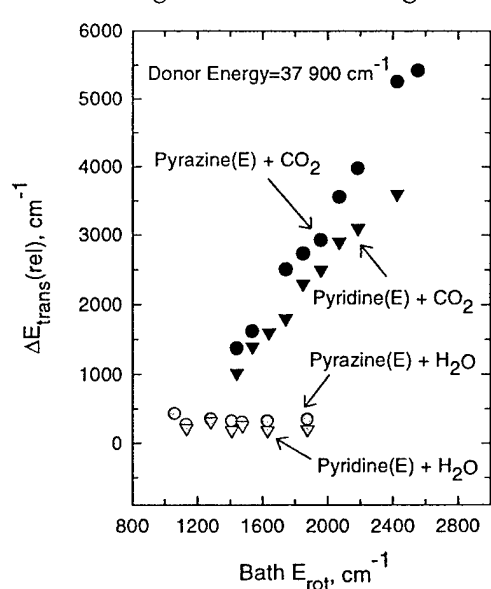
is measured using transient IR absorption. Their results are summarized below, where the energy gain profiles associated with the CO_2 (00^0_0) $J = 56\text{--}84$ states are shown as a function of pyrazine energy. Their data reveal some rather surprising results. Rather than a continuous increase in the CO_2 energy gain with increasing pyrazine energy, the energy transfer magnitude exhibits two plateau regions, separated by a stepwise increase in both rotation and translation at a pyrazine internal energy near $E \sim 36000\text{ cm}^{-1}$. The rate of energy transfer is essentially constant for pyrazine internal energies from 31000 to 36000 cm^{-1} , but shows a five-fold linear increase over the energy



range from 36000 to 41000 cm^{-1} . Thus large ΔE impulsive energy transfer becomes more important at higher internal energies, because the magnitude and the probability of energy transfer increase. In addition, Mullin has some very recent energy-dependent results for pyridine relaxation in the energy range 37000 to 41000 cm^{-1} . In this case, the observed CO_2 energy gain profiles are essentially constant and the energy transfer rate is also constant, much as is observed for pyrazine with $E=31000\text{--}34000\text{ cm}^{-1}$. This is extremely interesting in light of our results on the impact of donor complexity and suggests that for pyridine, the excited donor may be below the threshold for the onset of large ΔE energy transfer. At the present time, the source of our energy-dependent threshold is not fully understood, but this is one of the issues they hope to address in the future studies.

Mullin has also used transient IR absorption probing to investigate how donor energy content influences vibrational energy gain in CO_2 , which is known to occur via long-range near-resonant energy transfer. In this process, collisions excite CO_2 vibrational motion with almost no accompanying rotational or translational excitation. They have measured the energy dependence of the energy gain in the 00^0_1 (2349 cm^{-1}), 02^2_0 (2-quanta excitation of bend at 667 cm^{-1}), and $10^0_0r_1$ and $1^0_0r_2$ (Fermi mixed states of the symmetric stretch at 1270 and 1360 cm^{-1}) vibrational modes. In sharp contrast to the energy dependence for the (00^0_0) state, the rotational and translational energy gain profiles for the vibrationally excited states are not altered by the donor internal energy for the entire range investigated, $E=31000\text{--}42000\text{ cm}^{-1}$. Most surprisingly, they find that the probability (\sim once out of 120 collisions) for vibrational energy gain in CO_2 is also essentially unperturbed by the 11000 cm^{-1} variation in the pyrazine energy. It is quite interesting that the observed probability is very similar to that for the quintessential case of resonant vibrational energy transfer for small molecules at low energy, $\text{N}_2(1) + \text{CO}_2 \rightarrow \text{N}_2(0) + \text{CO}_2(00^0_1)$, which has an energy transfer probability of \sim once out of 70 collisions. Mullin's data suggest that long-range collisional relaxation of highly excited complex donors is not affected by the large amplitude vibrational dynamics that is believed to be associated with the highly excited donor. These data also indicate that as the donor internal energy is decreased, the near-resonant channel takes on increasing importance relative to the "supercollision" channel.

Energy gain in H_2O : the role of acceptor identity: Bulk energy loss measurements indicate that water is nearly always more efficient (by $\sim 50\%$) than CO_2 at quenching highly excited molecules. A logical conclusion might be that water removes larger amounts of energy from hot donors than does CO_2 .



Using an F-center laser to monitor appearance of individual rotational states of water, Mullin's group has measured the energy gain dynamics of this molecule following collisions with highly excited pyrazine and pyridine, prepared with $E \sim 38000\text{ cm}^{-1}$. Collisions with both donors result in scattered $\text{H}_2\text{O}(000)$ molecules that have a significant amount of rotational energy ($T_{\text{rot}}=920\text{ K}$ for pyrazine and $T_{\text{rot}}=770\text{ K}$ for pyridine) but low recoil velocities, shown in open symbols here. Strikingly, the amount of energy transferred to rotationally excited states of $\text{H}_2\text{O}(000)$ is only about 20% of that for $\text{CO}_2(00^0_0)$, which is shown as filled symbols for comparison. These results demonstrate that the great majority of $\text{H}_2\text{O}(000)$ supercollisions carry away significantly less energy

than do $\text{CO}_2(00^00)$ supercollisions. In addition, they have found that the energy gain *probabilities* for $\text{H}_2\text{O}(000)$ are comparable to those for $\text{CO}_2(00^00)$, accounting for only a few percent of all collisions. Thus, the enhanced quenching efficiency of water in bulk relaxation studies is not a result of the strong collisions seen in our experiments. The magnitude and partitioning of energy in the water supercollisions can be explained using a rotational shielding model in which the relatively rapid rotational motion of water favors collisions with the hydrogen atoms rather than the central oxygen. Thus, impulsive collisions result in torque on the water rather than recoil. Currently studies are underway in the Mullin labs to investigate the role of methyl substitution on the energy gain pathways of water.

Theoretical modeling using classical trajectory methods. Classical trajectory calculations have been used in the past decade to explore the source of supercollision relaxation. Schatz finds that supercollisions occur for the relaxation of hot CS_2 in a bath of Ar atoms and that the probability for these events is very small. Gilbert has seen evidence for impulsive collisions of Xe with excited azulene that are associated with direct encounters involving C-H stretches. He also observes a second type of collision in which the Xe atom skims across the azulene molecule, undergoing multiple encounters and picking up large amounts of translational energy. While this second type of collision is not considered a supercollision (because of the multiple hits), the two different mechanisms could not be distinguished in an experiment. Mullin's group would like to obtain similar insights into the ways that *polyatomic* quenchers gain energy through collisions. Luther and coworkers have performed interesting trajectory calculations on self-quenching of benzene that focussed on average quenching behavior, for which experimental data were available. In collaboration with David Coker of Boston University, Mullin has recently embarked on a theoretical project using classical trajectory calculations to explore collisional relaxation of high energy azabenzene in molecular baths. Their goal is to identify the nature of the collisions that result in the types of energy partitioning found in their state-resolved studies. Initially they have focussed on the pyrazine/ CO_2 system, for which they already have extensive experimental results. Based on an as yet unpublished potential that Luther has shared with us, Mullin and Coker have developed a simple model potential consisting of harmonic bond stretches and bends, together with a model torsional potential and a simple Lennard-Jones atom-atom intermolecular interaction between the highly excited ground state pyrazine and CO_2 molecules. The initial goal of this project has been to attempt to understand the large rotational and translational energy gains observed in the CO_2 bath. So far, they have reproduced correlation of large rotational angular momentum and recoil velocities in the scattered CO_2 molecules for the largest ΔE encounters with pyrazine and CO_2 . They are now attempting to identify the nature of the excited molecule's vibrations that are involved in these large ΔE energy exchanges. The potential model they have developed is flexible and they can explore the qualitative effect of adding longer ranged interactions in these studies. Their approach is to see if the state-resolved experimental results can be reproduced by varying the form of the model potential. Once this is observed, they will analyze the trajectories and explore the mechanism for the energy flow from the highly excited azabenzene. When this phenomenon is understood sufficiently, they will refine the potentials in order to reproduce the quantitative details of energy transfer. These details include a description of how the energy is partitioned in the bath molecule, how rapidly energy transfer occurs and at what internal energies molecular decomposition of the hot donor begins to be important. This approach will also be used to model energy transfer for other systems that they have studied experimentally, including the relaxation of other hot donors such as pyridine, 2-picoline and 2,6-lutidine, as well as collisional energy gain in water. In addition, since they will be using harmonic potentials to model vibrational motion, they can selectively excite individual normal modes in the excited

molecule and study the effects of non-randomized vibrational energy in the collisional energy transfer.

B. Publications resulting from ONR support

Research supported during this grant period has resulted in eight journal publications, one ACS symposium book (edited), and seven more journal articles in preparation.

1. Amy S. Mullin and George C. Schatz, editors, *Highly Excited Molecules: Relaxation, Reaction and Structure* (ACS Books, Washington, D.C. 1997).
2. Amy S. Mullin and George C. Schatz, "Dynamics of highly excited states in chemistry: An overview," in *Highly Excited Molecules: Relaxation, Reaction and Structure*, Amy S. Mullin and George C. Schatz, editors (ACS Books, Washington, D. C. 1997)
3. Mark C. Wall, Brian A. Stewart and Amy S. Mullin, "State-resolved collisional relaxation of highly vibrationally excited pyridine ($E_{\text{vib}}=38,000\text{ cm}^{-1}$) and CO_2 : Influence of a permanent dipole moment." *J. Chem. Phys.* **108**, 6185-6196 (1998).
4. Mark C. Wall and Amy S. Mullin, "Supercollision energy dependence: State-resolved energy transfer in collisions between highly vibrationally excited pyrazine ($E_{\text{vib}} = 37,900\text{ cm}^{-1}$ and $40,900\text{ cm}^{-1}$) and CO_2 ," *J. Chem. Phys.* **108**, 9658-9667 (1998).
5. Margaret Fraelich, Michael S. Elioff and Amy S. Mullin, "State-resolved studies of collisional quenching of highly vibrationally excited pyrazine by water: The case of the missing $V \rightarrow \text{RT}$ supercollision channel," *J. Phys. Chem.* **102**, 9761-9771 (1998).
6. Mark C. Wall, Andrew Lemoff* and Amy S. Mullin, "An independent determination of supercollision energy loss magnitudes and rates in highly vibrationally excited pyrazine with $E_{\text{vib}}= 36,000$ to $41,000\text{ cm}^{-1}$," *J. Phys. Chem.* **102**, 9101-9105 (1998).
7. Michael S. Elioff, Mark C. Wall, Andrew S. Lemoff* and Amy S. Mullin, "Observation of an energy threshold for large ΔE collisional relaxation of highly vibrationally excited pyrazine ($E_{\text{vib}}= 31,000$ to $41,000\text{ cm}^{-1}$) by CO_2 ," *J. Chem. Phys.* **110**, 5578-5588 (1999).
8. Margaret Fraelich, Michael S. Elioff, Rebecca L. Sansom* and Amy S. Mullin, "State-resolved collisional relaxation of highly vibrationally excited pyridine by H_2O : Role of strong electrostatic attraction in $V \rightarrow \text{RT}$ energy transfer," *J. Chem. Phys.* **111**, 3517-3525 (1999).
9. Mark C. Wall, Andrew Lemoff* and Amy S. Mullin, "Unraveling the energy dependence in large ΔE $V \rightarrow \text{RT}$ energy transfer: Separation of ΔE and probability in the collisional relaxation of highly vibrationally excited pyrazine ($E_{\text{vib}} = 36,000\text{ cm}^{-1}$ to $41,000\text{ cm}^{-1}$) by CO_2 ," *J. Chem. Phys.* **111**, 7373-7384 (1999).
10. Michael Elioff, Rebecca Sansom* and Amy S. Mullin, "Vibrational energy gain in the ν_2 bending mode of water via collisions with hot pyrazine ($E_{\text{vib}}=37900\text{ cm}^{-1}$): Insights into the dynamics of energy flow," *J. Phys. Chem. A* **104**, 10304-10311 (2000), Special Issue for C. Bradley Moore.
11. Michael S. Elioff, Andrew Lemoff,* Mark C. Wall, Emily Wilson, Amy Schneider,* Margaret Fraelich and Amy S. Mullin, "Energy dependence of long-range vibrational energy transfer from highly excited pyrazine ($E_{\text{vib}} = 33,000$ to $40,900\text{ cm}^{-1}$) to CO_2 ," manuscript in preparation
12. Ziman Li, Ekatarina Korobkova, Michael S. Elioff, Jeunghee Park, Andrew Lemoff,* Craig Rossi* and Amy S. Mullin, "Vibrational energy-dependence of large ΔE energy loss from highly excited pyridine ($E_{\text{vib}}= 37,000\text{ cm}^{-1}$ to $40,800\text{ cm}^{-1}$) through collisions with CO_2 ," manuscript in preparation
13. Jeunghee Park, Andrew Lemoff,* Lawrence Shum,* Kathryn Werner* and Amy S. Mullin, "The role of molecular complexity on relaxation via "strong" collisions: State-resolved

- quenching of highly vibrationally excited 2-picoline and 2,6-lutidine by CO₂," manuscript in preparation
14. Michael S. Elioff, Maosen Fang and Amy S. Mullin, "Methylation effects in state-resolved quenching studies of highly excited azabenzenes ($E_{\text{vib}} = 38000 \text{ cm}^{-1}$) with water," manuscript in preparation
 15. Michael S. Elioff, Maosen Fang, Joshua Neudel* and Amy S. Mullin, "Controlling energy transfer with rotational velocity: State-resolved quenching of vibrationally hot pyrazine ($E_{\text{vib}} = 38000 \text{ cm}^{-1}$) by collisions with HOD" manuscript in preparation
 16. Ekatarina Korobkova, Ziman Li, Lawrence Shum,* Kathryn Werner* and Amy S. Mullin, "State-resolved relaxation of hot pyrazine ($E_{\text{vib}} = 37900 \text{ cm}^{-1}$) by collisions with DCl: Influence of bath polarity and shape," manuscript in preparation
 17. Rebecca L. Sansom*, Sara Bonella, David F. Coker and Amy S. Mullin, "Quantum resolved quenching dynamics of hot pyrazine with CO₂: A classical trajectory study," manuscript in preparation.

Note: Research by undergraduates is featured in publications 6-13 and 15-17 as denoted by asterisks.

C. Human resources developed during the project period

<i>Graduate students</i>	Michael Elioff (PhD 2001), Emily Wilson (MS 1997), Maosen Fang (PhD candidate), Katya Korobkova (PhD candidate), Ziman Li (PhD candidate)
<i>Undergraduates</i>	Marc Kennedy (BA 1997, currently at the US Naval Academy), Andrew Lemoff (BA 1999, currently a PhD student in chemistry at University of California Berkeley), Craig Rossi (BA 1999), Rebecca Sansom (BA 2001), Amy Schneider (BA 1998, Wesleyan University), Lawrence Shum (BA 2000, currently employed at Harvard Medical School) and Kathryn Werner (BA 2000, currently a PhD student at Temple University), Joshua Neudel (BA 2001)
<i>Postdoctoral fellows</i>	Margaret Fraelich (currently a staff scientist at Infrared Technologies, Fort Worth, Texas) and Mark Wall (currently a staff scientist at Massachusetts Institute of Technology)
<i>Visiting scientists</i>	Jeunghee Park (Professor of Chemistry, Korea University) and Brian Stewart (Professor of Physics, Wesleyan University)

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May 8, 2001

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Greetings:

With this letter, I am submitting the final report for my Young Investigator Award,
N00014-96-1-0798.

With regards,

A handwritten signature in cursive script, appearing to read "Amy Mullin".

Amy S. Mullin